Voronoi Diagrams and a Numerical Estimation of a Quantum Channel Capacity

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Abstract. We give a new geometric interpretation of quantum pure states. Using Voronoi diagrams, we reinterpret the structure of the space of pure states as a subspace of the quantum state space. In addition to the known coincidence of some Voronoi diagrams for one-qubit pure states, we will show that even for mixed one-qubit states, as far as sites are given as pure states, the Voronoi diagram with respect to some distances — the divergence, the Bures distance, and the Euclidean distance — are all the same.

As to higher level pure quantum states, for the divergence, the Fubini-Study distance, and the Bures distance, the coincidence of the diagrams still holds, while the coincidence of the diagrams with respect to the divergence and the Euclidean distance no longer holds. That fact has a significant meaning when we try to apply the method used for a numerical estimation of a one-qubit quantum channel capacity to a higher level system.

1 Introduction

The movement of trying to apply quantum mechanics to information processing has given vast research fields in computer science [1]. Especially among them, the field which pursues the effectiveness of a quantum communication channel is called quantum information theory. Some aspect of quantum information theory is to investigate a kind of distance between two different quantum states. Depending on the situation, several distances are defined in quantum states. In quantum information geometry, the structure of those distances is of great interest [2, 3].

In classical information geometry, Onishi and Imai [4, 5] did a computational geometric analysis using a Voronoi diagram. A Voronoi diagram and a Delaunay triangulation are defined with respect to the Kullback-Leibler divergence, and are shown to be the extensions of the Euclidean counterparts. The Voronoi diagram is computed from an associated potential function instead of a paraboloid which is used in a Euclidean Voronoi diagram.

In this paper, we extend the Voronoi diagram in classical geometry to the quantum setting. In quantum information theory, there is a natural extension

of the Kullback-Leibler divergence, which is called a quantum divergence. We discuss a Voronoi diagram with respect to the quantum divergence, and analyze its structure.

For pure states in the space of one-qubit quantum states, the authors showed the coincidence of Voronoi diagrams with respect to some distances — the divergence, the Fubini-Study distance, the Bures distance, the geodesic distance and the Euclidean distance [6]. Here the diagram with respect to the divergence can be defined by taking a limit of the diagram in mixed states. As an application of this fact, we introduced a method to compute numerically the Holevo capacity of a quantum channel [7]. The effectiveness of this method is partially based on the coincidence of the diagrams. Moreover, also as to the diagrams in mixed states with sites given as pure states, we found the coincidence of some of them; the diagrams with respect to the three distances — the divergence, the Fubini-Study distance, and the Bures distance — coincide [8].

A natural question that arises after this story is "What happens in a higher level system?" For a higher level system, the diagrams with respect to the divergence and the Euclidean distance do not coincide anymore [9]. On the other hand, the diagrams with respect to the divergence, the Bures distance and the Fubini-Study distance still coincide for a higher level.

The rest of this paper is organized as follows. In Sect. 2, we give some definitions and prepare some mathematical tools. In Sect. 3, we give a theorem about a Voronoi diagram for one-qubit quantum states. In Sect. 4, we explain a method to compute the Holevo capacity and its relation to the proven theorem. In Sect. 5 and Set. 6, we extend the discussion of one-qubit Voronoi diagram to a higher level. Lastly we give a conclusion in Sect. 7. The latest result of our research is the latter half of Sect. 3 (Theorem 2) and Sect. 6. We give all the theorems without detailed proofs. The proofs will be given in the paper being prepared [8].

2 Preliminaries

2.1 Parameterization of quantum states

In quantum information theory, a *density matrix* is a representation of some probabilistic distribution of states of particles. A density matrix is expressed as a complex matrix which satisfies three conditions: a) It is Hermitian, b) the trace of it is one, and c) it must be semi-positive definite. We denote by $\mathcal{S}(\mathbb{C}^d)$ the space of all density matrices of size $d \times d$. It is called a *d-level system*.

Especially in a two-level system, which is often called a *one-qubit* system, the conditions above are equivalently expressed as

$$\rho = \begin{pmatrix} \dfrac{1+z}{2} & \dfrac{x-iy}{2} \\ \dfrac{x+iy}{2} & \dfrac{1-z}{2} \end{pmatrix}, x^2 + y^2 + z^2 \leq 1, \quad x, y, z \in \mathbb{R}. \tag{1}$$

The parameterized matrix correspond to the conditions a) and b), and the inequality correspond to the condition c). In this case, a density matrix correspond to a point in a ball. We call it a *Bloch ball.*

There have been some attempt to extend this Bloch ball expression to a higher level system. A matrix which satisfies only first two conditions, Hermitianness and unity of its trace, is expressed as:

$$\rho =
\begin{pmatrix}
\dfrac{\xi_1+1}{d} & \dfrac{\xi_d-i\xi_{d+1}}{2} & \cdots & & \dfrac{\xi_{3d-4}-i\xi_{3d-3}}{2} \\
\dfrac{\xi_d+i\xi_{d+1}}{2} & \dfrac{\xi_2+1}{d} & \cdots & & \dfrac{\xi_{5d-8}-i\xi_{5d-7}}{2} \\
\vdots & & \ddots & & \vdots \\
\dfrac{\xi_{3d-6}+i\xi_{3d-5}}{2} & \cdots & & \dfrac{\xi_{d-1}+1}{d} & \dfrac{\xi_{d^2-2}-i\xi_{d^2-1}}{2} \\
\dfrac{\xi_{3d-4}+i\xi_{3d-3}}{2} & \cdots & & \dfrac{\xi_{d^2-2}+i\xi_{d^2-1}}{2} & \dfrac{-\sum_{i=1}^{d-1}\xi_i+1}{d}
\end{pmatrix}, \quad \xi_i \in \mathbb{R}.$$

(2)

Actually, any matrix which is Hermitian and whose trace is one is expressed this way with some adequate $\{\xi_i\}$. This condition doesn't contain a consideration for a semi-positivity. To add the condition for a semi-positivity, it is not simple as in one-qubit case; actually we have to consider complicated inequalities [10, 11]. Note that this is not the only way to parameterize all the density matrices, but it is reasonably natural way because it is natural extension of one-qubit case and has a special symmetry.

Additionally our interest is a pure state. A pure state is expressed by a density matrix whose rank is one. A density matrix which is not pure is called a mixed state. A pure state has a special meaning in quantum information theory and also has a geometrically special meaning because it is on the boundary of the convex object. For one-qubit states, the condition for ρ to be pure is simply expressed as $x^2+y^2+z^2 = 1$. This is a surface of the Bloch ball. On the other hand, in general case, the condition for pureness is again expressed by complicated equations.

2.2 Some distances and the Holevo capacity

For two pure states ρ and σ, the Fubini-Study distance $d_{\mathrm{FS}}(\rho,\sigma)$ is defined by

$$\cos d_{\mathrm{FS}}(\rho,\sigma) = \sqrt{\mathrm{Tr}\,(\rho\sigma)}, \qquad 0 \leq d_{\mathrm{FS}}(\rho,\sigma) \leq \frac{\pi}{2}.$$

(3)

See Hayashi [12]. The Bures distance $d_{\mathrm{B}}(\rho,\sigma)$ [13] is defined by

$$d_{\mathrm{B}}(\rho,\sigma) = \sqrt{1 - \mathrm{Tr}\,(\rho\sigma)}.$$

(4)

Moreover, the Bures distance is also defined for mixed states. When ρ and σ are mixed states, their Bures distance is defined as

$$d_{\mathrm{B}}(\rho,\sigma) = \sqrt{1 - \mathrm{Tr}\,\sqrt{\sqrt{\sigma}\rho\sqrt{\sigma}}}.$$

(5)

Since Tr $\sqrt{\sqrt{\sigma}\rho\sqrt{\sigma}} = \text{Tr } \rho\sigma$ when ρ and σ are pure, this definition is consistent with the definition above for pure states.

The quantum divergence is one of measures that show the difference of two quantum states. The quantum divergence of the two states σ and ρ is defined as

$$D(\sigma||\rho) = \text{Tr } \sigma(\log \sigma - \log \rho). \tag{6}$$

Note that though this has some distance-like properties, it is not commutative, i.e. $D(\sigma||\rho) \neq D(\rho||\sigma)$. The divergence $D(\sigma||\rho)$ is not defined when ρ does not has a full rank, while σ can be non-full rank. This is because for a non-full rank matrix, a log of zero appears in the definition of the divergence. However, since $0 \log 0$ is naturally defined as 0, some eigenvalues of σ can be zero.

A quantum channel is the linear transform that maps quantum states to quantum states. In other words, a linear transform $\Gamma : M(\mathbb{C}; d) \rightarrow M(\mathbb{C}; d)$ is a quantum channel if $\Gamma(\mathcal{S}(\mathbb{C}^d)) \subset \mathcal{S}(\mathbb{C}^d)$.

The Holevo capacity [14] of this quantum channel is known to be equal to the maximum divergence from the center to a given point and the radius of the smallest enclosing ball. The Holevo capacity $C(\Gamma)$ of a 1-qubit quantum channel Γ is defined as

$$C(\Gamma) = \inf_{\sigma \in \mathcal{S}(\mathbb{C}^d)} \sup_{\rho \in \mathcal{S}(\mathbb{C}^d)} D(\Gamma(\sigma)||\Gamma(\rho)). \tag{7}$$

3   Voronoi Diagrams for One-qubit Quantum States

We define the Voronoi diagrams with respect to the divergences as follows.

$$V_D(v_i) = \bigcap_{i \neq j} \left\{ \sigma | D(\sigma||\rho(v_i)) \geq D(\sigma||\rho(v_j)) \right\},$$

$$V_{D^*}(v_i) = \bigcap_{i \neq j} \left\{ \sigma | D(\rho(v_i)||\sigma) \geq D(\rho(v_j)||\sigma) \right\}. \tag{8}$$

Note the quantum divergence is only defined for the mixed states. Actually, while $D(\rho||\sigma) = \text{Tr } \rho(\log \rho - \log \sigma)$ can be defined when an eigenvalue of ρ equals 0 because $0 \log 0$ can be naturally defined as 0, it is not defined when an eigenvalue of σ is 0. Here we show that this Voronoi diagram of mixed states can be extended to pure states. In other words, we prove that even though the divergence $D(\rho||\sigma)$ can not be defined when σ is a pure state, the Voronoi edges are naturally extended to pure states. In other words, we can define a Voronoi diagram for pure states by taking a natural limit of the diagram for mixed states. When we say "a Voronoi diagram with respect to divergence for pure states", it means a diagram obtained by taking a limit of a diagram for mixed states.

The following theorem shown in [9] characterize the Voronoi diagrams that appear on the sphere of one-qubit pure states.

Theorem 1. *For given one-qubit pure states, the following four Voronoi diagrams are equivalent for pure states:*

1. *the Voronoi diagram with respect to the Fubini-Study distance,*
2. *the Voronoi diagram with respect to the Bures distance,*
3. *the Voronoi diagram on the sphere with respect to the ordinary geodetic distance,*
4. *the section of the three-dimensional Euclidean Voronoi diagram with the sphere, and*
5. *the Voronoi diagram with respect to the divergences, i.e. V_D and V_{D^*}.*

Proof. See [9].

Note that generally the limit of V_D is meaningless because the diagram depends on how the sites converges. However, in a one-qubit system, since there is a special symmetry, we can think of a "natural" convergence of the sites. Actually just take the sites on the same sphere with its center at the origin, and converge the radius of the sphere to 1. In the theorem above, "the Voronoi diagram with respect to V_D" means the limit of the diagram obtained by such a convergence. Since that definition is only valid for a one-qubit system, for a higher level, only V_{D^*} is defined.

For mixed states, we found we can say the similar thing. We have the following theorem:

Theorem 2. *For given one-qubit pure states. the following Voronoi diagrams are equivalent for any states (including mixed states)*

- *the Voronoi diagram with respect to the Bures distance,*
- *the Euclidean Voronoi diagram with the sphere, and*
- *the Voronoi diagram with respect to the divergences, i.e. V_D and V_{D^*}.*

Proof. See [8].

4   Holevo Capacity for One-qubit Quantum States

Our first motivation to investigate a Voronoi diagram in quantum states is the numerical calculation of the Holevo capacity for one-qubit quantum states [7]. We explain its method in this section. In order to calculate the Holevo capacity, some points are plotted in the source of channel, and it is assumed that just thinking of the images of plotted points is enough for approximation. Actually, the Holevo capacity is reasonably approximated taking the smallest enclosing ball of the images of the points. More precisely, the procedure for the approximation is the following:

1. Plot equally distributed points on the Bloch ball which is the source of the channel in problem.
2. Map all the plotted points by the channel.
3. Compute the smallest enclosing ball of the image with respect to the divergence. Its radius is the Holevo capacity.

In this procedure, Step 3 uses a farthest Voronoi diagram. That is the essential part to make this algorithm effective because Voronoi diagram is the known fastest tool to seek a center of a smallest enclosing ball of points.

However, when you think about the effectiveness of this algorithm, there might arise a question about its reasonableness. Since the Euclidean distance and the divergence are completely different, Euclideanly uniform points are not necessarily uniform with respect to the divergence. We gave partial answer to that problem by Theorem 1. At least, on the surface of the Bloch ball, the coincidence of Voronoi diagrams implies that the uniformness of points with respect to Euclidean distance is equivalent to the uniformness with respect to the divergence.

5 Voronoi Diagrams for Three or Higher Level Quantum States

In [9], the authors showed that the coincidence of the divergence-Voronoi diagram and the Euclidean Voronoi diagram which happens in one-qubit case never occurs in a higher level case. In this section, we explain the outline of the proof described in [9]. To show that fact, it is enough to look at some section of the diagrams with some (general dimensional) plane. If the diagrams do not coincide in the section, you can say they are different.

Suppose that $d \geq 3$ and that the space of general quantum states is expressed as (2), and let us think the section of it with a $(d+1)$-plane:

$$\xi_{d+2} = \xi_{d+3} = \cdots = \xi_{d^2-1}. \tag{9}$$

Then the section is expressed as:

$$\rho = \begin{pmatrix} \frac{\xi_1+1}{d} & \frac{\xi_d-i\xi_{d+1}}{2} & & & \text{\Large 0} \\ \frac{\xi_d+i\xi_{d+1}}{2} & \frac{\xi_2+1}{d} & & & \\ & & \ddots & & \\ & & & \frac{\xi_{d-1}+1}{d} & \\ \text{\Large 0} & & & & \frac{-\sum_{i=1}^{d-1}\xi_i+1}{d} \end{pmatrix}. \tag{10}$$

Under that condition, we obtain the the expression of the boundary as follows:

$$(\eta_d - \tilde{\eta}_d)\xi_d + (\eta_{d+1} - \tilde{\eta}_{d+1})\xi_{d+1} + \frac{4(\eta_1 - \tilde{\eta}_1)\left(\xi_1 - \frac{d-2}{2}\right)}{d^2} = 0. \tag{11}$$

The detailed process to obtain this equation is described in [9].

Moreover, (11) tells us a geometric interpretation of this boundary. We obtain the following theorem:

Theorem 3. *On the ellipsoid of the pure states which appears in the section with the $(d+1)$-plane defined above, if transfered by a linear transform which maps the ellipsoid to a sphere, the Voronoi diagram with respect to the divergence coincides with the one with respect to the geodesic distance.*

Proof. See [9]

Now we work out the Voronoi diagram with respect to Euclidean distance. Under the assumption above, the Euclidean distance is expressed as

$$
\begin{aligned}
d(\sigma, \rho) &= (\eta_1 - \xi_1)^2 + (\eta_2 - \xi_2)^2 + (\eta_d - \xi_d)^2 + (\eta_{d+1} - \xi_{d+1})^2 \\
&= 2(\eta_1 - \xi_1)^2 + (\eta_d - \xi_d)^2 + (\eta_{d+1} - \xi_{d+1})^2,
\end{aligned} \tag{12}
$$

and we get the equation for boundary as

$$
\begin{aligned}
d(\sigma, \rho) - d(\tilde{\sigma}, \rho) = -4(\eta_1 - \tilde{\eta}_1)\xi_1 - 2(\eta_d - \tilde{\eta}_d)\xi_d - 2(\eta_{d+1} - \tilde{\eta}_{d+1})\xi_{d+1} + 2(\eta_1^2 - \tilde{\eta}_1^2) \\
+ (\eta_d^2 - \tilde{\eta}_d^2) + (\eta_{d+1}^2 - \tilde{\eta}_{d+1}^2) = 0. \quad (13)
\end{aligned}
$$

By comparing the coefficients of ξ_1, ξ_d, and ξ_{d+1}, we can tell that the boundaries expressed by (11) and (13) are different.

6   Bures distance and Fubini-Study Distance

Although the diagrams with respect to the divergence and the Euclidean distance are different as shown in the previous section, for the divergence, the Bures-distance and the Fubini-Study distance, the coincidence of diagrams which holds for one-qubit states also holds for a higher level. It is stated as follows:

Theorem 4. *In a general level quantum system, for pure states, the following diagrams are equivalent:*

- *diagram with respect to the divergence*
- *diagram with respect to Fubini-Study distance*
- *diagram with respect to Bures distance*

The equivalence between the Fubini-Study diagram and the Bures diagram is obvious because

$$
d_{\mathrm{B}}(\rho, \sigma) \leq d_{\mathrm{B}}(\rho, \tilde{\sigma}) \iff \mathrm{Tr}\,\rho\sigma \geq \mathrm{Tr}\,\rho\tilde{\sigma} \iff d_{\mathrm{FS}}(\rho, \sigma) \leq d_{\mathrm{FS}}(\rho, \tilde{\sigma}) \tag{14}
$$

Hence the only thing to show is the coincidence between the diagram by Bures distance and the diagram by divergence. The rest of the proof is described in [8].

7   Concluding Remarks

We showed that in the one-qubit system, the Voronoi diagrams with respect to some distances are the same. Among them, coincidence of the divergence-Voronoi diagram and the Bures-Voronoi diagram for pure states especially plays an important role in a numerical calculation of a capacity of a quantum communication channel.

Our next target is a capacity evaluation of a higher level quantum communication channel. However, as we showed in this paper, the theoretical support for

the one-qubit numerical capacity estimation — the coincidence of the divergence-Voronoi diagram and Bures-Voronoi diagram — does not hold in a higher level. On the other hand, we showed that the divergence-, Bures-, and Fubini-Study-Voronoi diagram are all the same even for a higher level.

The facts we showed have a negative impact for a higher-level numerical capacity estimation. The naive extension of the method for one-qubit quantum states is found to be not efficient for a higher level. Nevertheless, our geometrical analysis for quantum states has contributed to a further interpretation of the space of quantum states. Our next work is a numerical capacity estimation especially for three-level system, and we believe the analysis in this paper will be helpful for that objective.

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